Lecture Slides for
Matrix Calculus

Winter 2022
Alan Edelman/Steven Johnson
11am-1pm MWF
• Lectures: January 10, 12, 14, 19, 21, 24, 26, 28
• 11am-1pm virtual, short break around noon
• Two Homeworks: Released Wednesday due following Wednesday on canvas, 11:59pm due
• 3 Credits
• Linear Algebra such as 18.06 assumed

Some demos and hw may use julia (no experience assumed, though most LinAlg classes at MIT use a little Julia already)
Where does matrix calculus fit in?

- **MIT 18.01**: Scalar or Single Variable Calculus
- **MIT 18.02**: Vector or Multivariable Calculus

Perhaps an ideal world might go Scalar, Vector, Matrix, Higher Dimensional Arrays…
(0 dimensional, 1 dimensional, 2 dimensional…)
(e.g. size(scalar)=[], size(vector)=[n], size(matrix)=[m,n],...)
(some programming language do not implement this fully)

Why now?

- In the last decade or two, the role of linear algebra has taken on larger importance in lots of areas including Machine Learning, Statistics, Engineering, etc.
- Warning: googling Matrix Calculus may only give a small view of the full range of the mathematics that we hope to cover example what is the derivative of $X^2$ when $X$ is a square matrix? Should it be $2X$? (It’s not). What about $X^{-1}$? -$X^{-2}$? (Not quite).
Applications: Machine Learning
buzzwords: parameter optimization
stochastic gradient descent, autodiff, backpropagation

Matrix Calculus for Machine Learning

As Machine Learning deals with data in higher dimensions, understanding algorithms with knowledge of one and two variable calculus is cumbersome and slow. If someone asks for the derivative of $x^2$, without a second you will tell its $2x$, without using the first principles-definition of differentiability. Here, I will provide some tips and tricks to perform matrix calculation just like the differentiation of $x^2$. 

Notes on Matrix Calculus for Deep Learning

Deep learning is an exciting field that is having a great real-world impact. This article is a collection of notes based on 'The Matrix Calculus You Need For Deep Learning' by Terence Parr and Jeremy Howard.
Applications: Physical Problems

**Topography-optimized aircraft wing**

~ $10^9$ parameters

Goal: maximize stiffness under external loads, utilizing limited amount of material
→ Light but strong
→ 100s tonnes of fuel saving

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**Topology optimization with fluid dynamics**

(A) High Re flow, velocity magnitude
(B) Low Re flow, velocity magnitude

Switching flow channels for high vs. low viscosity

Used with permission.

Key point is that if you have *any* complicated calculation with lots of parameters, you can compute gradient (sensitivity) of a scalar output $g(u)$ with respect to every parameter with roughly *one* additional calculation.

Enabling factor for large-scale optimization in machine learning

*$g$ = loss function, $u$ = network outputs, $p$ = network weights & other parameters*, statistics, finance, and many other fields.
Applications: Data Science & Multivariable Statistics

Derivative of a Matrix: Data Science Basics

**Derivative of a Matrix**

\[
\frac{d}{dx} kx = A = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}
\]

\[
\frac{d}{dx} kx^2 =
\]
The Role of Automatic Differentiation

Typical differential calculus classes are mostly symbolic calculus:

- Students learn to do what mathematica/wolfram alpha readily can do

For a small portion of the class, some numerics may show up

- approximate $f'(x)$ by finite differences $(f(x+\epsilon)-f(x)) / \epsilon$ or $(f(x+\epsilon)-f(x-\epsilon)) / 2\epsilon$
- e.g. students and professors think that “sin” is actually computed using Taylor series

Today’s automatic differentiation is neither of these two things. It is more in the field of the computer science topic of compiler technology than mathematics.

However the underlying mathematics is interesting! We will learn about this in this class.
Everything is easy with scalar functions of scalars

- The derivative of a function of one variable is a function of one variable
- The linearization of a function has the form \((y-y_0)=f'(x_0)(x-x_0)\)

Other notations (sometimes confusing \(x\) and \(x_0\)):

- \(\delta y = f'(x) \delta x\)
- \(dy = f'(x)dx\)
- \(f(x)-f(x_0) = f'(x_0)(x-x_0)\)
- \(df = f'(x)dx \quad \leftarrow \text{this one is preferred}\)

- Numerics are fairly trivial:
Numerical Example of what’s going on in the previous slide

Suppose \( f(x) = x^2 \) with \( (x_0,y_0)=(3,9) \) and \( f'(x_0)=6 \)

\[
\begin{align*}
  f(3.0001) &= 9.00060001 \\
  f(3.00001) &= 9.0000600001 \\
  f(3.000001) &= 9.000006000001 \\
  f(3.0000001) &= 9.00000060000001 \quad (\text{Notice that } \Delta y = 6 \Delta x) \\
  f(3 + \Delta x) &\approx 9 + \Delta y = 9 + 6 \Delta x \quad (\Delta y = f'(x_0) \Delta x)
\end{align*}
\]

\[
f(x) - f(3) \approx 6 (x-3) \quad \text{← linearization of } x^2 \text{ at } x=3 \text{ is the “multiply by 6” function}
\]

We write:

\[
\begin{align*}
  dy &= f(x_0+dx) - f(x_0) \quad \text{where } dy = f'(x_0)dx \quad \text{or } f(x_0+dx) = f(x_0) + f'(x_0)dx \\
  \text{I think of } dx \text{ and } dy \text{ as really small numbers; in math they are called } \text{infinitesimal}. \\
  \text{In rigorous mathematics, one takes limits.}
\end{align*}
\]
http://www.matrixcalculus.org/

Notation: Elementwise vector or matrix product. We will use $x.*y$, they use $x \odot y$

- $[2,3].*[10,11] = [20,33]$
- $\text{trace}(A) = \text{tr}(A) =$ the sum (a scalar) of the diagonal elements of matrix $A$

Some limitations:
- matrixcalculus.org will not display derivatives that involve more than 2 dimensions:
  - e.g. a derivative of a matrix with respect to a vector or a matrix

If we differentiate a scalar function of a matrix

Answer is a matrix: $-2X' (Y-X\theta)$

We will teach you to solve problems like this!
Format of the first derivative: The explicit notation

<table>
<thead>
<tr>
<th>input ↓ \ output →</th>
<th>scalar</th>
<th>vector</th>
<th>matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>scalar</td>
<td>scalar</td>
<td>vector (e.g. velocity)</td>
<td>matrix</td>
</tr>
<tr>
<td>vector</td>
<td>vector (gradient) (arguably a row vector though often a column vector in beginning classes)</td>
<td>matrix (Jacobian matrix)</td>
<td>higher order array</td>
</tr>
<tr>
<td>matrix</td>
<td>matrix</td>
<td>higher order array</td>
<td>higher order array</td>
</tr>
</tbody>
</table>

Format of the first derivative: implicit view: The linear operator

dx^3 = 3x^2 dx  scalar in, scalar out  (multiply the infinitesimal scalar dx by 3x^2 )

d(x'x) = 2x' dx  scalar in, vector out (take the dot product of the infinitesimal vector dx with the vector 2x)

dX^2 = XdX + dX X matrix in, matrix out  (multiply the infinitesimal matrix dX by matrix X on each side and add)

You will learn to do any of these in great detail – the purpose of this slide is just to plant the notion of linearization.
Let’s check the linearization numerically

\[ f(x) = x^T x \]

\[ x_0 = [3; 4] \quad f(x_0) = x_0^T x_0 = 25 \]

\[ dx = [0.001; 0.002] \quad (3.001)^2 + (4.002)^2 = 25.022005 \]

\[ 2x_0^T dx = 2 [3; 4]^T [0.001; 0.002] = 0.022 \]

Notice that \( f(x_0 + dx) \approx f(x_0) + 2x_0^T dx = 25 + 0.022 \)
Matrix and vector product rule

\[ d(AB) = (dA)B + A(dB) \] is still correct but generally the products do not commute.

However if \( x \) is a vector

\[ d(x^T x) = dx^T x + x^T dx \] and since vector dot products commute (\( a \) dot \( b \) is \( b \) dot \( a \)), we in this special case can write \( d(x^T x) = (2x)^T dx \).

Example: \( x=[1;2;3;4] \); \( dx=\text{rand}(4)/100000; \)

\((x+dx)' (x+dx) - x'x \) # this is \( d(x'x) \)

\((2x)^T dx \) # this is approximately the same as \( d(x'x) \)

Note: the way the product rule works for vectors and matrices is that transposes “go for the ride”

Examples:

1. \( d(u^T v) = du^T v + u^T dv \) but note \( du^T v = v^T du \) because dot products commute
2. \( d(uv^T) = duv^T + udv^T \)
For the explicit form we want all derivatives of outputs w.r.t. to all inputs.

How many parameters are needed?

Answer:
Second derivatives (a few words for starters)

Explicit form: The second derivative of a scalar valued function of a vector is represented explicitly as a symmetric matrix known as the Hessian of the function.

Implicit form: All second derivatives are what is known in advanced linear algebra as a quadratic form (or a symmetric bilinear form).